

## A Compact, Generalized Equation of State for Polar and non-Polar Fluids

L. Sun,<sup>S</sup> S. B. Kiselev, and J. F. Ely<sup>C</sup>

*Department of Chemical Engineering  
Colorado School of Mines, Golden, CO 80401, U.S.A.  
jely@mines.edu*

Development of an accurate generalized equation of state (EOS) for different substances has been of great interest for many years. High accuracy Bender- and MBWR-type equations have been individually fit for a wide variety of fluids [1,2]. However, these equations do not work well for substances that are not well defined in the experimental database, and can be numerically unstable when fit to systems with limited data. Recently, Span [3] used a simultaneous optimization algorithm to develop two compact equations of state with only 12 terms, one for polar fluids and one for non-polar fluids. Although these two short EOS give very good representations of the thermodynamic properties of polar and non-polar fluids separately, the need for the unified EOS for both groups of fluids remains.

In this work, we have developed a simultaneous optimization algorithm for the structure of a generalized EOS, which is based on the simulated annealing algorithm. Secondly, we applied this algorithm to develop a universal EOS for both, polar and non-polar fluids. Finally, using QSAR techniques, we have developed a method of predicting the parameters of the universal equation using molecular descriptors. The resulting equation predicts the thermodynamic surface of both types of fluids practically with the same accuracy as the corresponding individual equations developed for polar and non-polar fluids reported by Span [3].

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- [2] B. Platzer, Dissertation (in German), Univ. Kaiserslautern, Kaiserslautern, Germany (1990).
- [3] R. Span, *Multiparameter Equations of State* (Springer-Verlag, Berlin, Germany, (2000).